MOLECULAR PHYSICS

VOLUME 11

Printed and Published by
TAYLOR & FRANCIS LTD
RED LION COURT, FLEET STREET, LONDON, E.C.4

Copyright © TAYLOR & FRANCIS LTD

CONTENTS OF VOLUME 11

NUMBER 1

Page

Tautomerie von 2-Picolylketonen. II. Die N.M.R.-Spektren von 2-Picolylisopropylketon und 2-Picolylphenylketon. G. Klose und K. Arnold 1

The electronic spectra of diphenyl and its sterically hindered derivatives. R. Grinter 7

Préionisation et prédissociation dans la dissociation des molécules triatomiques par impact électronique. F. Fiquet-Fayard et P. M. Guyon 17

On the theory of hypochromism. G. N. Fowler 31

N.M.R. studies of electrolytes in binary solvent mixtures. I. 10 : 1 aqueous mixtures of acetone, N,N-dimethylformamide, dimethylsulphoxide, dioxane, ethanol, and N-methylformamide. Anthony Fratiello and Don Paul Miller 37

The electron resonance of ground state triplets in liquid crystal solutions. H. R. Falle, G. R. Luckhurst, H. Lemaire, Y. Marechal, A. Rassat and P. Rey 49

Unstable intermediates: an electron spin resonance study of Ag_2^+. L. Shields and M. C. R. Symons 57

R-matrix theory of molecular collisions. L. Blum 63

Fluorine chemical shifts in aromatic systems. G. L. Caldow 71

Semi-empirical molecular orbital energy levels of XeF_4. Walter A. Yeranos 85

Research Notes

Molionic lattices. Jan Kommandeur and Gerard T. Pott 93

First and second quantum deviations of the second virial coefficient for the Kihara potential. R. D. Weir 97

NUMBER 2

Calculation of the singlet–triplet splitting of the dinegative ions of some aromatic molecules. J. N. Murrell and A. Hinchliffe 101

Variational method for molecular re-arrangement collisions. L. Blum .. 105

Comments on the application of group theory to the analysis of high-resolution N.M.R. spectra. C. M. Woodman 109

Calculations of chemical shifts. Part I. ^{19}F, ^{1}H and ^{13}C chemical shifts of alkanes and cycloalkanes. J. Feeney, L. H. Sutcliffe and S. M. Walker 117

Calculations of chemical shifts. Part II. ^{19}F shifts of fluorinated cyclopentenes. J. Feeney, L. H. Sutcliffe and S. M. Walker 129

Page

Calculations of chemical shifts. Part III. ^{19}F shifts of interconverting fluorinated cyclohexenes. J. FEENEY, L. H. SUTCLIFFE and S. M. WALKER 137

Calculations of chemical shifts. Part IV. ^{19}F shifts of 1,2,4-trichloroheptafluorocyclohexene evidence for axial substitution. J. FEENEY, L. H. SUTCLIFFE and S. M. WALKER 145

Relative validity of the valence bond theory and of the molecular orbital theory for description of conjugated hydrocarbons. H. LOOYENGA 153

Electron spin resonance spectrum of HCN^- in alkali halide matrices. K. D. J. ROOT, M. C. R. SYMONS and B. C. WEATHERLEY 161

Kerr dispersion in alkali metal vapours. L. L. BOYLE and C. A. COULSON 165

Biradicals of the dibenzoylmethane dianion. H. VAN WILLIGEN and S. I. WEISSMAN 175

Perturbation approach to the proton spin coupling in the ethane fragment. P. CHANDRA and P. T. NARASIMHAN 189

Zero-field splittings in aromatic hydrocarbons. II. Calculations with π-electron wave functions including overlap and extensive configuration interaction. COLIN THOMSON 197

NUMBER 3

The structure of Coppinger's radical and its orientation within a cluster of a liquid crystal. G. R. LUCKHURST 205

An SCF calculation of mono-substituted benzenes. P. KNOWLTON and W. R. CARPER.. 213

Molecular orbital calculations for aromatic carbonyl compounds. B. CANTONE, F. GRASSO and S. PIGNATARO 221

Thermal conductivity of binary and ternary mixtures of krypton, argon and helium. R. S. GAMBHIR and S. C. SAXENA 233

On the calculation of spin densities. FRANK E. HARRIS 243

E.S.R. Study of the free radicals produced by the γ-irradiation of pyridine. C. DAVID, G. GEUSKENS, A. VERHASSELT, P. JUNG and J. F. M. OTH .. 257

Classification of the states of non-rigid molecules. B. J. DALTON 265

The dependence of the fluorine–electron Overhauser effect upon the correlation time of the molecular motion in liquids. R. A. DWEK, J. G. KENWORTHY, J. A. LADD and R. E. RICHARDS 287

RESEARCH NOTES

The electron resonance spectrum of perinaphthenyl dissolved in a liquid crystal. H. R. FALLE and G. R. LUCKHURST 299

The magnitude and sign of the directly-bonded ^{13}C–^{29}Si spin–spin coupling constant. K. A. MCLAUCHLAN 303

NUMBER 4

Page

The theory of double bond fixation in conjugated hydrocarbons. G. BINSCH, E. HEILBRONNER and J. N. MURRELL 305
Linewidth variations in the electron resonance spectrum of the trinitromethyl radical dianion. A. HUDSON, C. LAGERCRANTZ and G. R. LUCKHURST .. 321
Proton and fluorine N.M.R. spectra of fluorobenzene. S. MOHANTY and PUTCHA VENKATESWARLU 329
Introduction of the electron repulsion into the molecular orbital wave function. H. LOOYENGA 337
Phosphorescence of substituted benzenes and their lowest triplet states. K. KIMURA and H. TSUBOMURA 349
Untersuchung der weitreichenden Kernspinkopplung über fünf Bindungen in planaren Kohlenwasserstoffen. H. FRISCHLEDER und G. BÄR .. 359
Molecular multipole moments. DANIEL E. STOGRYN and ALEX P. STOGRYN 371

RESEARCH NOTES

Re-assignment of P.M.R. spectrum of tris(diethylphenylphosphine) complexes of Ir^{III} and Rh^{III}. E. W. RANDALL and D. SHAW 395
Dimerization of gaseous nitric oxide. ROBERT L. SCOTT 399

ERRATUM

Dimerization of gaseous nitric oxide (correction). E. A. GUGGENHEIM .. 403

NUMBER 5

Forces in the benzene crystal. I. The lattice energy of crystalline benzene. K. BANERJEE and L. SALEM 405
Steady state and transient Overhauser effect in systems of three spins. D. F. S. NATUSCH, R. E. RICHARDS and D. TAYLOR 421
The effect of solvents on the chemical shift of fluorine nuclei in aromatic compounds. J. W. EMSLEY and L. PHILLIPS 437
Diagrammatic perturbation theory of multiphoton transitions. R. WALLACE 457
Rotational isomerism. II. A calculation of the solvent dependence of the conformational equilibria in substituted ethanes and its application to N.M.R. spectra. R. J. ABRAHAM, L. CAVALLI and K. G. R. PACHLER .. 471
The crystal and molecular structure of B-trimethylborazole. K. ANZENHOFER 495

RESEARCH NOTE

Possible organic superconductor. LIONEL SALEM 499

Erratum. K. A. MCLAUCHLAN 503
Erratum. ROBERT L. SCOTT. 503

NUMBER 6

Page

Determination of the relative signs of spin coupling constants from the temperature dependence of N.M.R. spectra. J(H–C–C≡C–CH) R. FREEMAN 505

Deuteron spin lattice relaxation in benzene, bromobenzene, water and ammonia. J. G. POWLES, M. RHODES and J. H. STRANGE 515

The electron spin resonance spectrum and electronic structure of the radical-anion of 1,8-bisdehydro-14-annulene. N. M. ATHERTON, R. MASON and R. J. WRATTEN 525

The limitations of generalization in sub-spectral analysis of N.M.R. spectra. P. DIEHL and D. TRAUTMANN 531

^{14}N chemical shifts in primary and secondary amides. P. HAMPSON and A. MATHIAS 541

On high temperature susceptibilities of Heisenberg model ferromagnetics and anti-ferromagnetics. K. PIRNIE, P. J. WOOD and J. EVE 551

The concept of intramolecular energy transfer in the theory of uni-molecular reactions. MILAN ŠOLC 579

Proton magnetic relaxation in dilute solutions of paramagnetic ions. H. PFEIFER, D. MICHEL, D. SAMES and H. SPRINZ 591

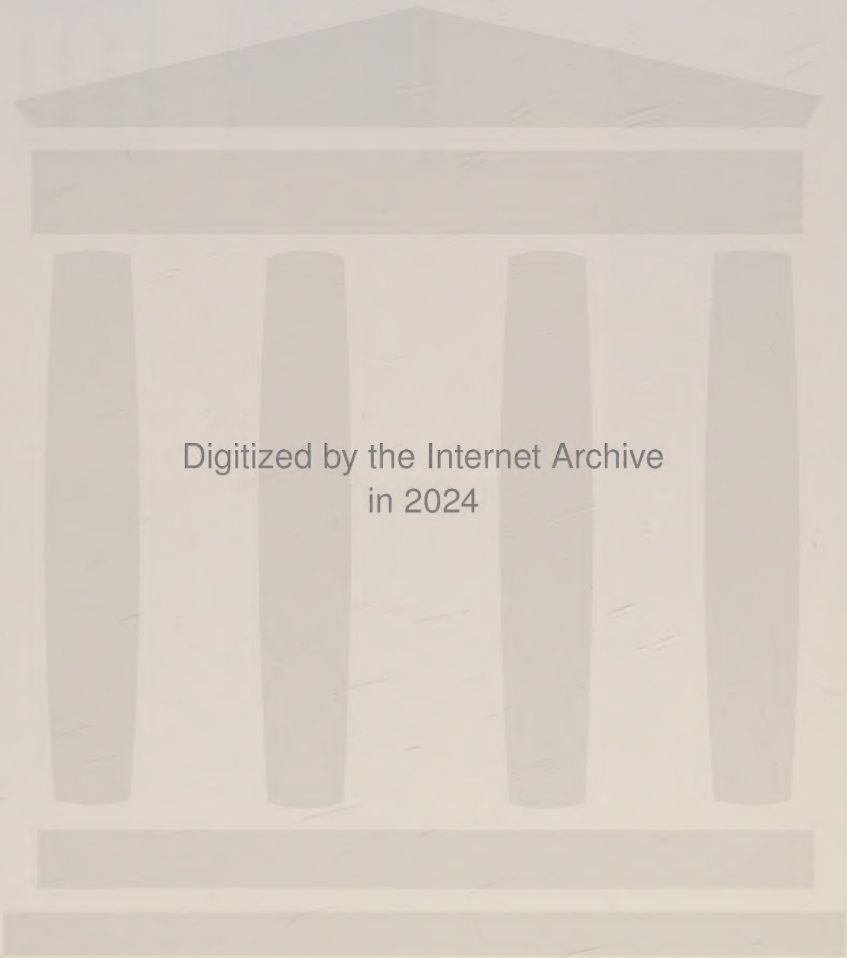
RESEARCH NOTES

An N.M.R. study of N,N-dimethylformamide complexes. ANTHONY FRATIELLO, RONALD SCHUSTER and DON PAUL MILLER 597

E.S.R. study of gamma irradiated binary mixtures of pyridine and methanol. C. DAVID, G. GEUSKENS, A. VERHASSELT, P. JUNG and J. F. M. OTH 599

A simple formula for some nuclear spin–spin coupling constants. W. T. DIXON 601

Index of authors (with the titles of papers) 605



Digitized by the Internet Archive
in 2024

https://archive.org/details/molecular-physics_1966_11_contents